

META-MODELS FOR PREDICTING BLOOD BRAIN BARRIER PENETRATION BASED ON SIMPLE PHYSICOCHEMICAL DESCRIPTORS

ABSTRACT OF THE INVENTION

- 5 Descriptor based models, employing at least two descriptors, predict activities of compounds under consideration. Those activities may be biology-based activities such as the ability of the compound to cross the blood brain barrier. In one example, the model predicts a compound's solubility, its ability to be absorbed in the intestine, and its ability to cross the blood brain barrier. The descriptors of interest are typically
- 10 physicochemical properties of the whole molecule. Examples include a log P or log D, molecular weight or related size-based descriptors, the number of hydrogen bond donors and/or hydrogen bond acceptors, formal charge, lipophilicity, and the like.

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